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A "numerical microscope" for plasma physics

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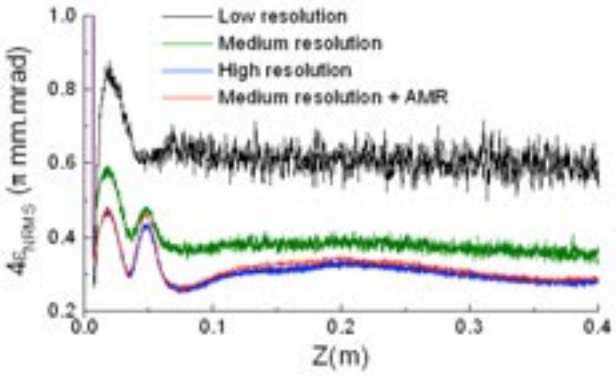
A “numerical microscope” for plasma physics

A new simulation capability developed for heavy-ion inertial fusion energy research will accelerate plasma physics and particle beam modeling, with application to multiple fields of scientific and industrial interest.

Computer simulation of plasmas is important to a number of fields in both science and industry, including particle accelerators (because beams of charged particles are non-neutral plasmas), high-power vacuum tubes, and advanced microcircuit fabrication and plasma processing of materials. Researchers at the Heavy Ion Fusion Virtual National Laboratory (HIF-VNL) and LBNL's Computational Research Division have prototyped key elements of a new approach that uses adaptive-mesh refinement to increase both the speed and the accuracy of these simulations.



In this computational experiment, the benchmark for accuracy was a high-resolution grid (blue), but results almost indistinguishable from it (red) were achieved at about one-fourth the computing cost by using a medium resolution grid and adaptive mesh refinement. These results were substantially better than those obtained from a medium grid without adaptive mesh refinement (green) and much better than results from a coarse grid (black). This study of a simple system bodes well for reconciling accuracy and feasibility in large, complex systems, such as heavy-ion accelerators for inertial fusion energy.

One of the main approaches for computer simulation of plasmas requires integrating two simulation elements – a model of the electromagnetic field, and computation of the behavior of a collection of particles. In these simulations, the electromagnetic field is calculated at a finite number of “mesh points.” Usually the grid is uniform, but when the system being modeled is large and must be examined on several spatial scales at once, this presents a dilemma: a fine uniform mesh would require too much computing power and a coarse uniform mesh would overlook key details; yet non-uniform grids complicate the particle tracking and field solution.

An end-to-end model of beam behavior in the kind of accelerator needed for inertial fusion energy spans nine orders of magnitude in size – some crucial details have to be modeled at the micron level, and the whole complex could be a kilometer or more long. To address this scale disparity, researchers turned to a technique called the adaptive mesh refinement method, which has been applied successfully in such areas as computational fluid dynamics. Adaptive mesh refinement applies a closer-spaced mesh only to the areas that need finer resolution at any given moment.

The challenge until now has been the integration of these two powerful but disparate techniques--a discrete representation of the particles and a mesh-refined representation of the electromagnetic fields--into a single computer program. This is the goal of the research being reported. The final product will be the first of its kind, and will have applicability far beyond inertial fusion energy, wherever plasma simulation is used.

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Further information:
Extended summary of work and images: [put in a link to pdf] (nnn k)

[UI2.003] "Application of Adaptive Mesh Refinement to Particle-in-Cell Simulations of Plasmas and Beams" Abstract: http://www.aps.org/meet/DPP03/baps/abs/S2320003.html

Reporters seeking additional information should contact David Harris, 301-209-3238, harris@aps.org or Ben Stein, 301-209-3091, bstein@aip.org.

The HIF-VNL (a joint endeavor of Lawrence Berkeley and Lawrence Livermore National Laboratories and the Princeton Plasma Physics Laboratory) and its work toward the goal of inertial-fusion power plants based on beams of heavy ions, are described further at http://hif.lbl.gov/

A “numerical microscope” for plasma physics

A new simulation capability developed for heavy-ion inertial fusion energy research will accelerate plasma physics and particle beam modeling, with application to multiple fields of scientific and industrial interest.

Computer simulation of plasmas is important to a number of fields, some of which may not immediately come to mind when one thinks of plasma physics. These fields include particle accelerators (because beams of charged particles are non-neutral plasmas), high-power vacuum tubes, advanced microcircuit fabrication, and plasma processing of materials. Modeling plasmas requires calculation of both particle behavior and the electromagnetic fields in the system. Researchers at the Heavy Ion Fusion Virtual National Laboratory (HIF-VNL) and LBNL's Computational Research Division have prototyped key elements of a new approach that uses adaptive-mesh refinement to increase both the speed and the accuracy of these simulations.

One of the main approaches for computer simulation of plasmas consists of following the trajectories of “macroparticles” that interact with each other and their environment via the electromagnetic field (A macroparticle usually represents many actual particles; tracking all individual physical particles is rarely done, due to computational expense and the success of the macroparticle approach.) In these simulations, the electromagnetic field is calculated at a finite number of “mesh points.” Usually the grid is uniform, but when the system being modeled is large and must be examined on several spatial scales at once, this presents a dilemma: a fine uniform mesh would require too much computing power and a coarse uniform mesh would overlook key details (imagine a weather prediction model for an area that has mountains and plains – the mountains require a finer mesh because the details are more abundant and important.); yet non-uniform grids complicate the particle tracking and field solution.

Modeling beam behavior in an accelerator is one of many problems of that class, where the system is large and yet some parts of it are full of important fine detail. An end-to-end model of beam behavior in the kind of accelerator needed for inertial fusion energy spans nine orders of magnitude in size – some crucial details have to be modeled at the micron level, and the whole complex could be a kilometer or more long. To address this scale disparity, researchers are turning to a technique called the adaptive mesh refinement method, which has been applied successfully in such areas as computational fluid dynamics. Adaptive mesh refinement uses regular gridding for simplicity but applies a closer-spaced mesh to the areas that need finer resolution at any given moment. A good model with adaptive mesh refinement not only serves as a “numerical microscope” that lets researchers zoom in on areas of special interest, but actually offers a more accurate model of the system behavior.

The challenge until now has been the integration of these two powerful but disparate techniques--a discrete representation of the particles and a mesh-refined representation of the electromagnetic fields--into a single computer program. This is the goal of the research being reported. The key issues have been identified; for example, errors at the edge of refined areas in which the forces are calculated on a finer scale must not be allowed to introduce significant errors into the computed particle motion. Such issues, as well as the efficacy of the merged method on real problems, are being studied in detail using prototype codes.

One such prototype, built into the HIF accelerator code WARP, has been used to study and validate the method on the simulation of a particle-beam source. Results of a series of runs in reduced dimensionality, which illustrate the effectiveness of mesh refinement on this problem, are shown in Fig. 1. It shows how the use of mesh refinement in this case reduced computer time and memory requirements by almost a factor of four. Higher gains (factors of 1000 or more) have been realized in initial studies of the behavior of the head of the ion beam as it emerges from its source. That calculation used a special set of one-dimensional non-uniform refinement patches covering the emission region, where extreme particle density gradients are present.

Typical gains of a factor of ten or more are also expected when the ability to track macroparticles is added to a fully three-dimensional package called Chombo, currently under development at LBNL. A view of a field solution given by Chombo is shown in Fig. 2. The final product will consist of the improved Chombo package, complete with the means of linking it to existing particle simulation codes. It will be the first of its kind and will have applicability far beyond inertial fusion, wherever plasma simulation (or particle-field simulation for other purposes) is used.

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P. McCorquodale, P. Colella, D. P. Grote, J.-L. Vay, “A Node-Centered Local Refinement Algorithm for Poisson's Equation in Complex Geometries',” in preparation for submission to the Journal of Computational Physics.

J.-L. Vay, P. Colella, P. McCorquodale, B. Van Straalen, A. Friedman, D.P. Grote, “Mesh Refinement for Particle-In-Cell Plasmas Simulation: Application and Benefits for Heavy Ion Fusion", *Laser and Particle Beams* (2002), **20**, 569.

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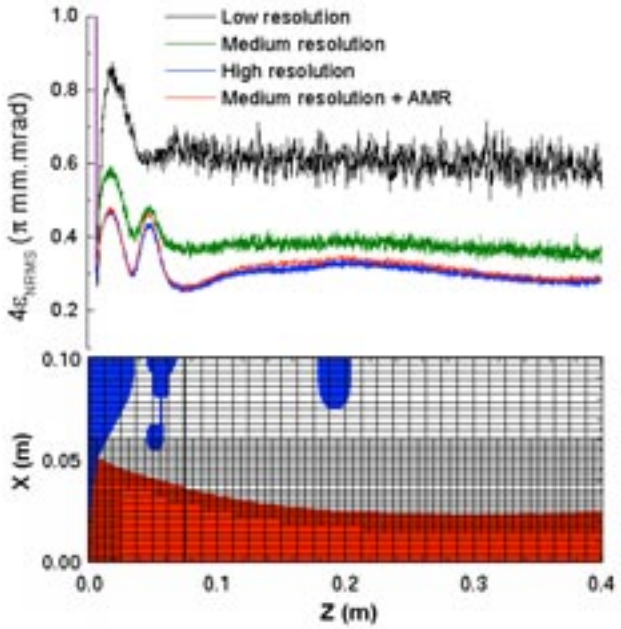

Figure 1. Simulation of a charged-particle beam source. This study of a simple system bodes well for reconciling accuracy and feasibility in large, complex systems, such as heavy-ion accelerators for inertial fusion energy.

Top: The beam emittance (a figure of merit for beam quality – the lower the better) is shown versus distance Z. In this computational experiment, the benchmark for accuracy was a high-resolution grid (blue), but results almost indistinguishable from it (red) were achieved at about one-fourth the computing cost by using a medium resolution grid and adaptive mesh refinement. These results were substantially better than those obtained from a medium grid without adaptive mesh refinement (green) and much better than results from a coarse grid (black).

Bottom: The beam injector structure is shown in blue. The beam (red) is emitted from the left and propagates to the right. The black lines denote the mesh: a higher resolution is used around the emission surface and at the edge of the beam.

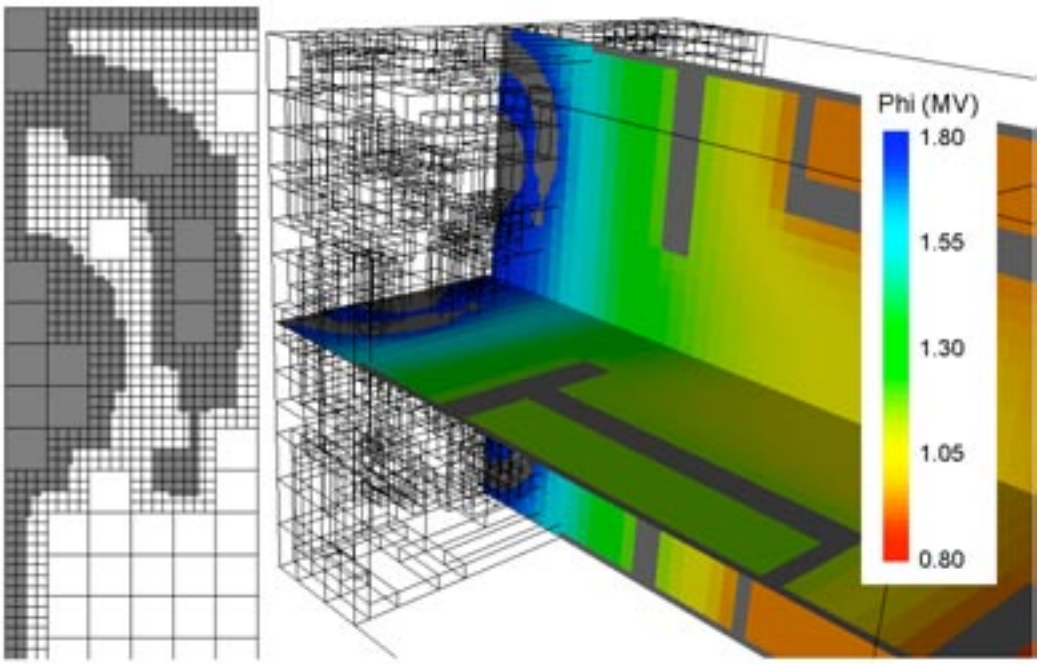

Figure 2
Three-dimensional solution of the field potential in the front end of an accelerator, as given by Chombo. A slice with the actual meshing (left) shows that the regions close to the boundaries of conductors (grey) are described with a fine mesh, while the interiors of conductors and regions of vacuum, less critical with regard to fine detail, are covered with coarser meshes.
The picture on the right shows a three-dimensional rendering that includes two orthogonal slices of the solution (with the magnitude of the electrostatic potential shown colored, and conductors in grey) and the edges of the different domains containing finer mesh spacing (in this case, mesh refinement covered the conductor edges only in the area surrounding the source). This field model is now being combined with the capability to track a large set of discrete particles, by linking Chombo to existing particle codes. This linkage is now working in a simplified prototype implementation, with coupling to WARP's 3-D model. The resulting novel research tool will have applications well beyond its roots in heavy-ion inertial fusion energy.

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